Lecture 1: Introduction to R

15.S60 Software Tools for Operations Research

Jerry Kung
MIT Operations Research Center
jkung@mit.edu

January 6, 2015

Outline

Introduction

Why use R?

- Free, widely-used language for data analysis
- Many packages available for statistics, machine learning
- 6000+ packages and counting; constantly being updated
- Can be used for scripting, data manipulation and analysis, and visualization

15.S60 (2015)

Today:

- Default environment (other GUIs exist: RStudio, rattle, Rcmdr)
- Scripting, basic data manipulation
- Packages: `rpart`, `caTools`, `randomForest`, `e1071`

15.S60 (2015)

Today:

- Default environment (other GUIs exist: RStudio, rattle, Rcmdr)
- Scripting, basic data manipulation
- Packages: `rpart`, `caTools`, `randomForest`, `e1071`

Lectures 2 and 3 also on R:

- Thursday (1/8): Data Wrangling by Clark Pixton and Evan Fields
- Tuesday (1/13): Visualization by Angie King

Resources and References

Official download: http://cran.us.r-project.org

- Also has documentation and FAQs
- Current version: `R 3.1.2 "Pumpkin Helmet"`

Other helpful sites:

- http://www.statmethods.net
- http://www.ats.ucla.edu/stat/dae/
- http://cran.r-project.org/doc/contrib/usingR.pdf
- http://www.rseek.org
- http://zoonek2.free.fr/UNIX/48_R/all.html

Outline

Outline

Logistic Regression

- Used for binary classification (e.g., predict whether or not a passenger survived)
- Uses a logistic function to predict the probability of a class:

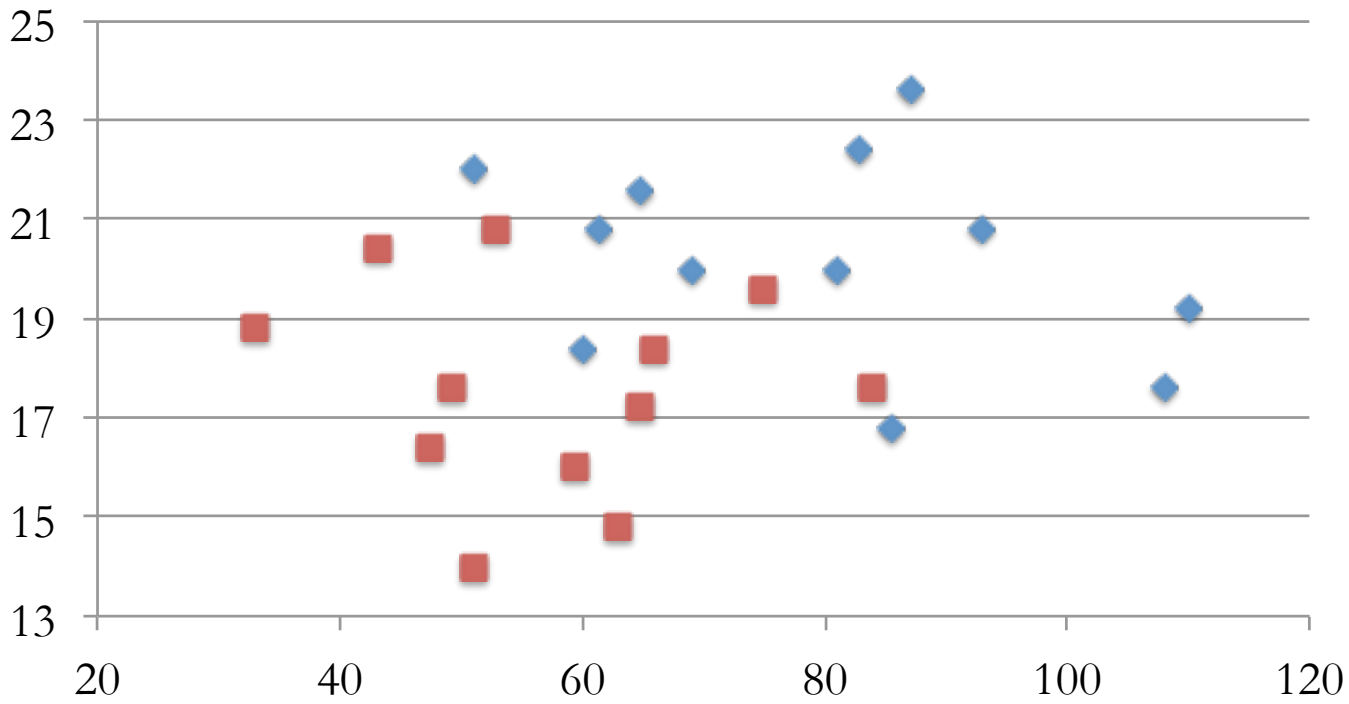
$$\mathbb{P}(\hat{y} = 1) = \frac{1}{1+e^{-(b_0+b_1x_1+\cdots+b_kx_k)}}$$

- Think about the term in the exponent as a linear regression; the logistic function then translates the estimate from the linear regression to a value between 0 and 1
- We then use a threshold value on the output of the logistic function
  - Often, this value is 0.5, meaning that we predict the class with the higher probability
  - Sometimes other threshold values may be more appropriate

Outline

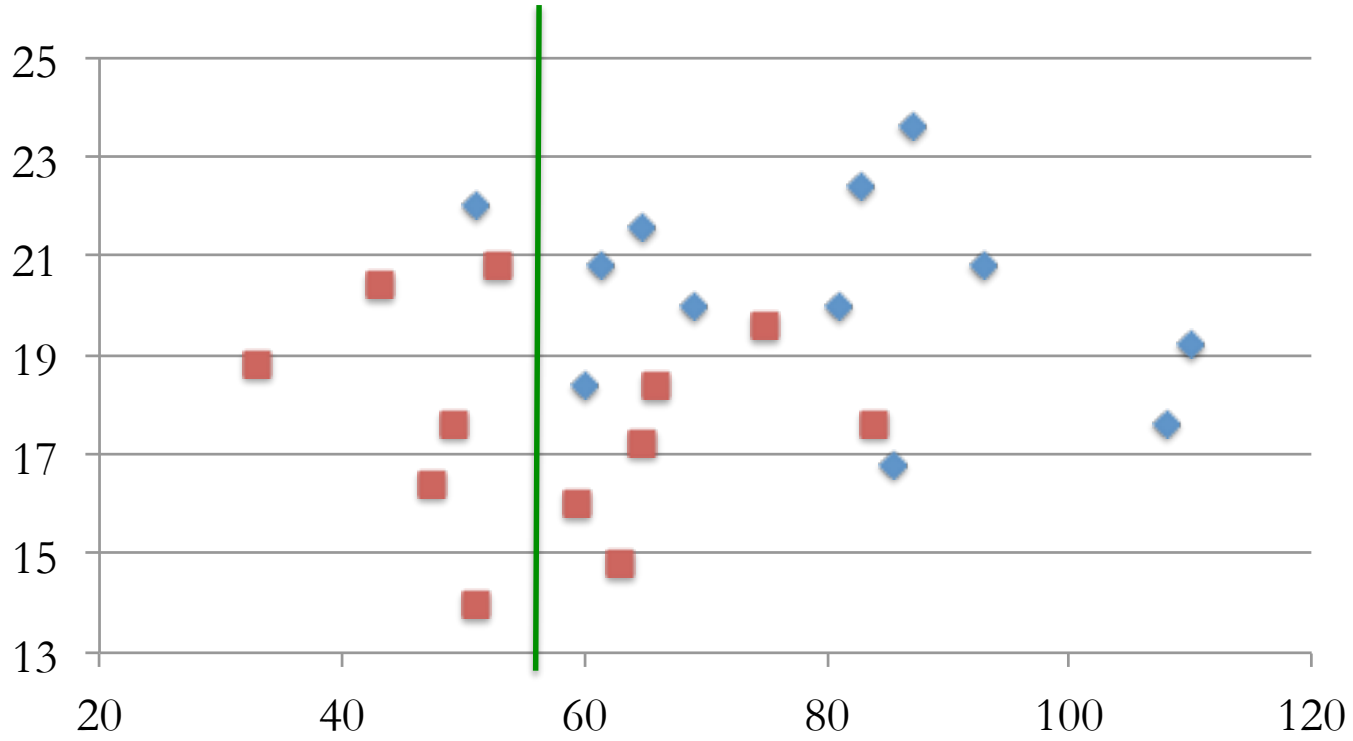
Classification and Regression Trees (CART)

- Make sequential splits on independent variables (e.g., was the passenger male? if yes, then consider age; if no, then consider class, and so on)
- Splits are made to make the "buckets" as "pure" as possible, in a greedy fashion



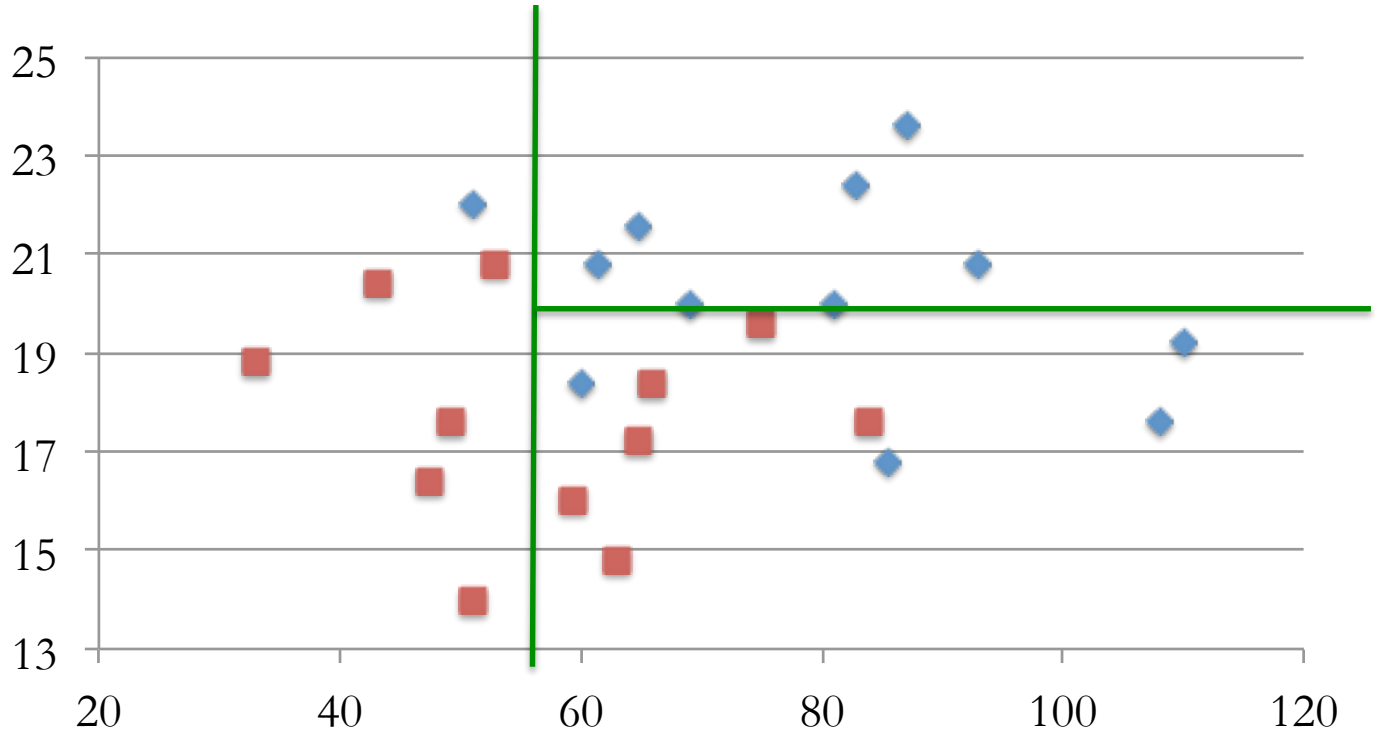
Classification and Regression Trees (CART)

- Make sequential splits on independent variables (e.g., was the passenger male? if yes, then consider age; if no, then consider class, and so on)
- Splits are made to make the "buckets" as "pure" as possible, in a greedy fashion



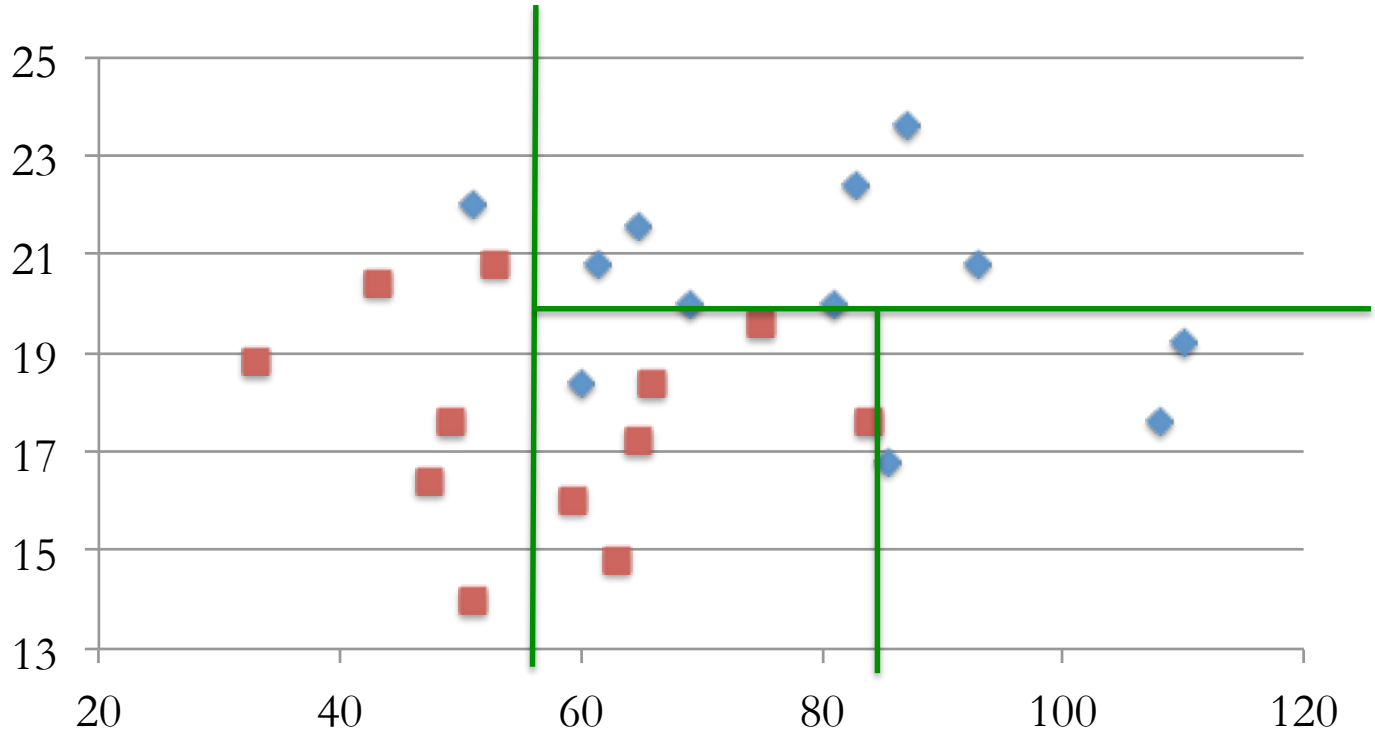
Classification and Regression Trees (CART)

- Make sequential splits on independent variables (e.g., was the passenger male? if yes, then consider age; if no, then consider class, and so on)
- Splits are made to make the "buckets" as "pure" as possible, in a greedy fashion



Classification and Regression Trees (CART)

- Make sequential splits on independent variables (e.g., was the passenger male? if yes, then consider age; if no, then consider class, and so on)
- Splits are made to make the "buckets" as "pure" as possible, in a greedy fashion



Classification and Regression Trees (CART)

- You can usually build a tree that fits the data exactly (except when two identical data points have differing classifications)
- Thus, we have to limit the power of the algorithm so that we don't overfit (strong performance on training data, but poor ability to generalize to test data and beyond)
  - `minbucket` requires each terminal leaf to have at least some number of points
  - `minsplit` will require a minimum number of points in a bucket before a split can be made
  - Can also limit the number of splits

Classification and Regression Trees (CART)

When might CART perform poorly?

Classification and Regression Trees (CART)

- Predictions made by CART trees can be multi-class categorical (e.g., yes or no; red, green, or blue, etc.). In this case, the prediction for a test data point is just the label of the majority of the points in that "bucket"
- Predictions can also be continuous (e.g., price, distance, etc.). In this case, the prediction for a test data point is just the average of the points in that "bucket"

Random Forest

- The random forest algorithm builds many CART trees that are uncorrelated
- For each CART tree, select only a subset of the data points on which to regress
- When making splits, only choose a subset of attributes that are permitted to be split upon (changes at each iteration of splits)
  - Defaults in R (which can be changed using `mtry`) are $\sqrt{m}$ for classification and $\frac{m}{3}$ for regression
- Prediction is the majority "vote" for classification and the mean of all trees for continuous outcomes

Outline

Types of Clustering

- Hierarchical (Agglomerative) Clustering
  - Each data point starts out as its own cluster. Then merge based on a given criterion until there is only one cluster remaining.
  - No need to specify the number of clusters, since you can visualize the hierarchy.
- K-means Clustering
  - Begin by specifying the centroids of k clusters. Assign each data point to the nearest cluster. Then re-center the resultant clusters and iterate.
  - Less computationally intensive than hierarchical clustering, so better for larger data sets.
- Many other types of clustering as well

Distance Metrics

- In order for us to cluster data points, we need to define a notion of distance between data points.
  - Today, we will use Euclidean distance (L_2 norm)
  - Manhattan (L_1 norm) and Maximum coordinate (L_{inf} norm) are common as well
  - Often is highly sensitive to scale (we can normalize by subtracting the mean and dividing by the standard deviation)
- We also need to define distances between two clusters.
  - Today, we will use centroid distance
  - Maximum and minimum cluster distances can be used as well

Hierarchical Clustering vs. K-means

- Advantages of Hierarchical Clustering:
  - No need to specify number of clusters in advance (use dendrograms to visualize)
  - Clusters are nested (you can see the hierarchy)
- Advantages of K-means Clustering:
  - Faster (important for large data sets)
  - Less influenced by choice of distance metric

Outline

Support Vector Machines

- At a high level, SVMs determine a decision boundary that maximizes the "margin" (which, roughly, is the distance from the boundary to the support vectors)
- The objective is to maximize this margin, while the constraints are to obey the labels on the points
- A nonlinear optimization problem, but can be solved efficiently (if interested, see Wikipedia article on SVMs; also refer to Lecture 6, taught by Miles Lubin)
- Using kernels, decision boundaries can be extended to polynomials and beyond (Gaussian, or radial basis, kernels can be constructed so that any training set can be classified correctly)

Outline

Thanks for listening!

- Special thanks to Allison O'Hair
- Solutions can be found at Git
  `https://github.com/joehuchette/OR-software-tools-2015`
- Please fill out feedback forms!
- Any questions? Feel free to e-mail `jkung@mit.edu`